



The statistical ensemble of q -deformed hyperbolic modified Pöschl-Teller potential for certain diatomic molecules through Euler-Maclaurin approach

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Abstract

The statistical properties are essentially needed to understand the macroscopic behaviours of atomic molecules, which is a crucial aspect of physics and chemistry research. In this work, q -deformed hyperbolic modified Pöschl-teller was used to obtain the statistical properties of H_2 , HCl , LiH , and CO using the energy eigenvalues that were gotten from the potential. The Nikiforov-Uvarov approach was used to elucidate the Schrödinger equation using the potential, while the partition functions were obtained through the Euler-MacLaurin technique. The result shows that both the partition functions and each of the statistical properties increase with an increase in the Boltzmann factor. The analytical results of vibrational internal energy, vibrational entropy, vibrational free energy, and vibrational specific heat capacity were obtained for the limit $0 < q \leq 1$. The study comes up with a new way to predict how potential deformation will affect the thermodynamic properties of diatomic molecules and the existence critical temperature which explain the phase transition of the diatomic particles. It also gives us useful information about the statistical properties of diatomic molecules, which helps us understand how they behave at the macro level. This is a big step forward for molecular physics.

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1. Introduction

Quantum group (QG) and quantum algebra (QA) have been investigated by both Physicists and mathematicians during the past decades. These fields had captivated the interest of people, especially during the initiation of q -deformed harmonic oscillator. QG and QA hidebound unpredicted application to theoretical physicists [1–3]. From a mathematical perspective, q -deformation in algebra can be related to Lie algebras, which is

a perfect example of Hopf algebras. Lie algebra is obtained whenever the parameter of deformation q tends to 1, the q -analogue of the harmonic oscillator in realisation of QA has instituted much work on this topic [4–6].

Lately, the theory of potential deformation in quantum mechanics (QM) has become a topic of fascination for some decades, and it has applications in several fields of Physics because of its application in different areas, such as q -deformed harmonic oscillator [7], q -deformed modified Pöschl-Teller potential [8], classical and quantum q -deformed physical system [9], q -deformed Tamm-Donco oscillator [10], de-

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formed Pöschl-Teller-like and some solvable potentials [11], q-deformed fermionic oscillator algebra [12], q-deformed Morse potential [1], and lastly fermionic q-deformation [13].

The interrelationship between atoms in diatomic molecules is of greater impact to atomic and molecular physics, which can be described by the potential of contention. It is one of the realistic harmonic potential models, which is well used to depict vibrational motion of diatomic molecules. In the numerical approach, the potential has been written in forms of SU(2) group, which was developed to compare experimental data and Dunham expansion for different diatomic molecules [14–20]. Polyatomic and Diatomic particles can be treated by changing their temperature from zero to pinch of thermal dissociation of their thermodynamic functions, using an analytical approach.[14, 21–27].

The vibrational partition function, which is of great significance to both engineering and chemical Physics can be achieved through the summation of its energy spectrum from definition; molecular vibrational particle function can be calculated by the totality of all the available energy levels of the system. Some explicit measures have been taken to obtain the vibrational partition function for molecular potential energy models for both polyatomic and diatomic molecules [13, 28–35]. The aim of this research is to calculate the statistical properties and some thermodynamic properties in terms of deformation parameter (q) using the Euler-Maclaurin approach [1, 2, 4, 13].

The organisation of the paper: In section 2, one-dimensional eigenvalue solution of The potential was obtained. In Section 3, the potential vibrational partition functions and consequently, the basic thermodynamic functions such as free energy, internal energy, entropy, and specific heat capacity were derived. In Section 4, the conclusion is given.

2. The Schrödinger equation in one dimension under the influence of the potential

The time independent Schrödinger equation under the influence of q-deformed hyperbolic modified Pöschl-Teller potential [8, 11]:

$$V(r) = -\frac{\hbar^2 (\eta^2 - 1/4)}{2m \cosh_q^2(\alpha r)}, \quad (1)$$

can be written as

$$\left[\frac{d^2}{dr^2} - \left(\frac{\eta^2 - 1/4}{\cosh_q^2(\alpha r)} \right) + \frac{2mE}{\hbar^2} \right] \Psi(r) = 0, \quad (2)$$

where η indicate the dissociation parameter, α represent the range parameter, m denote the reduced mass of the molecule, and $E_{n,l} = E_n$. Applying the deformation hyperbolic functions [1, 32, 33]:

$$\begin{aligned} \sinh_q y &= \frac{1}{2}(\exp^y - q \exp^{-y}), \\ \cosh_q y &= \frac{1}{2}(\exp^y + q \exp^{-y}), \cosh_q y = \frac{\sinh_q y}{\tanh_q y} \end{aligned} \quad (3)$$

and

$$\begin{aligned} \tanh_q y &= \frac{1}{\coth_q y}, \cosh_q^2 y = q + \sinh_q^2 y, \\ \frac{d \cosh_q y}{dy} &= \sinh_q y, \frac{d \sinh_q y}{dy} = \cosh_q y, \end{aligned} \quad (4)$$

we have

$$\int \cosh_q^2 y dy = q \tanh_q y, \& \frac{d \coth_q y}{dy} = \frac{-q}{\sinh_q^2 y}. \quad (5)$$

By substituting new variables: $\nu = \sqrt{\frac{-2mE}{\alpha^2 \hbar^2}}$ and $\xi = \frac{(\eta^2 - 1/4)}{\alpha^2}$ and using a new parameter $z = \tanh_q(\alpha r)$, equation (2) turns

$$\left\{ \frac{d}{dz} \left[(1 - z^2) \frac{d}{dz} \right] + \left[\frac{\xi}{q} - \frac{\nu^2}{1 - z} \right] \right\} \Psi(z) = 0. \quad (6)$$

Substituting $\Psi(z) = (1 - z^2)^{\frac{\nu}{2}} f(z)$ in equation (6), we obtain:

$$\begin{aligned} (1 - z^2) f''(z) - 2z(\nu + 1) f'(z) \\ + \left[\frac{\xi}{q} + \frac{\nu(\nu + 2)z^2}{(1 - z^2)} - \nu + \frac{3\nu z^2}{1 - z^2} \right] f(z) = 0. \end{aligned} \quad (7)$$

Equation (7) is in form of hypergeometric differential equation, of the solution [13]:

$$\Psi_n^q = N^q (1 - z^2)^{\frac{\xi}{2}} {}_2F_1 \left(-n, -n + 2w, -n + w + \frac{1}{2}; \frac{1 - z}{2} \right), \quad (8)$$

where ${}_2F_1 \left(-n, -n + 2w, -n + w + \frac{1}{2}; \frac{1 - z}{2} \right)$ are the hypergeometric polynomials of degree n and $w = \sqrt{\frac{1}{4} + \frac{\xi}{q}}$. The corresponding non-relativistic q-deformed eigenvalues read

$$E_n = -\frac{\alpha^2 \hbar^2}{2m} \left[\left(n + \frac{1}{2} \right) - w \right]^2. \quad (9)$$

$\frac{dE}{dn} = 0$ can be used to obtain the maximum value of n_{max} , where n_{max} is the maximum vibrational principal quantum number, so we have

$$n_{max} = w - \frac{1}{2}. \quad (10)$$

3. One-dimensional thermal properties of diatomic molecules under the influence of the potential

3.1. Methods

The summation of all available vibrational energy levels of the potential can be used in calculating the vibrational partition functions. The partition function Z of the potential at limited temperature, T is obtained via Boltzmann factor, β [3]:

$$Z = \sum_{n=0}^{\infty} \exp^{-\beta(E_n - E_0)}, \quad (11)$$

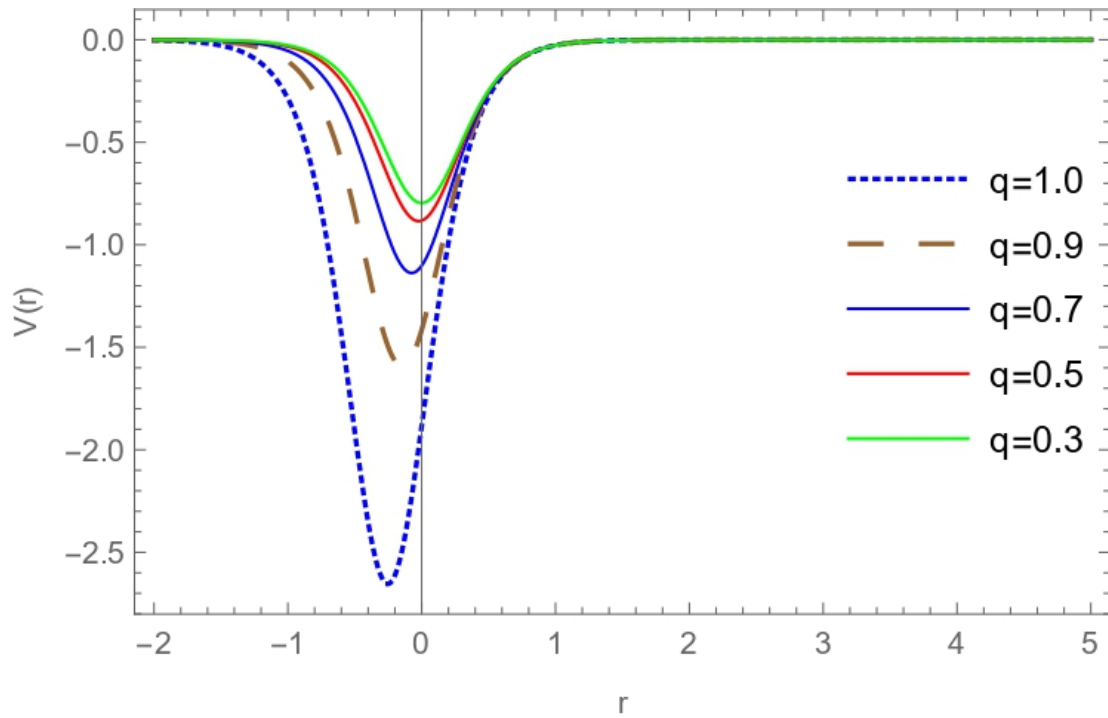


Figure 1. Variation of the potential for some values of q ($0 < q < 1$).

where $\beta = \frac{1}{k_B T}$ and k_B denote the Boltzmann constant. The Euler-Maclaurin formula for equation (11) is written as [1, 10, 13]:

$$\sum_{\eta=0}^{\infty} f(\eta) = \int_0^{\infty} f(\xi) d\xi + \frac{1}{2} f(\xi) d\xi + \sum_{q=1}^{\infty} \frac{B_{2q}}{(2q)!} f^{(2q-1)}(0), \quad (12)$$

where

$$Z = \sum_{\eta=0}^{\infty} f(\eta).$$

B_{2p} represent the Bernoulli numbers, order $(2q-1)$ is the derivative of $f^{(2q-1)}$. $q = 3$, and with $B_2 = \frac{1}{6}$ and $B_4 = -\frac{1}{30}$, the partition function Z for HCl can be written as:

$$\begin{aligned} Z(\beta, q, a) = & \frac{1}{2} - \frac{2.87266 \times 10^{23} \left(\frac{1}{2} - \sqrt{\frac{1}{4} + \frac{4.61908a^2}{q}} \right) \beta}{a^2} \\ & + \frac{1}{720} \left[\frac{-3.56495 \times 10^{49} \left(\frac{1}{2} - \sqrt{\frac{1}{4} + \frac{4.61908a^2}{q}} \right) \beta^2}{a^4} \right. \\ & \left. + \frac{4.09636 \times 10^{73} \left(\frac{1}{2} - \sqrt{\frac{1}{2} + \frac{4.61908a^2}{q}} \right)^3 \beta^3}{a^6} \right] \\ & - \left[6.75036 \times 10^{-13} e^{-\frac{1.45045 \times 10^{-25} \left(1.7236 \times 10^{24} - 3.4472 \times 10^{24} \sqrt{\frac{1}{4} + \frac{4.61908a^2}{q}} \right) \beta}{a^2}} \right] \\ & \times \left(6.56429 \times 10^{11} - 1.31286 \times 10^{12} \sqrt{\frac{1}{4} + \frac{4.61908a^2}{q}} \right) \\ & \times \text{Erf} \left(\sqrt{\frac{\left(6.56429 \times 10^{11} - 1.31286 \times 10^{12} \sqrt{\frac{1}{4} + \frac{4.61908a^2}{q}} \right)^2 \beta}{a^2}} \right) \\ & \div \left(\sqrt{\frac{6.56429 \times 10^{11} - 1.31286 \times 10^{12} \sqrt{\frac{1}{4} + \frac{4.61908a^2}{q}}}{a^2}} \right) \beta \end{aligned}$$

where Erf represent error function and $a = \frac{1}{\alpha}$.

The vibrational internal energy, free energy, entropy and specific heat of the potential are defined, respectively, as:

$$U = -\frac{d}{d\beta} \ln Z, \quad (13)$$

$$F = -\frac{1}{\beta} \ln Z, \quad (14)$$

$$S = \ln Z - \beta \frac{d \ln Z}{d\beta}, \quad (15)$$

and,

$$C = \beta^2 \frac{d^2}{d\beta^2} \ln Z. \quad (16)$$

3.2. Applications for few diatomic molecules

The results and the physical implication of the problem are discussed and concluded on the following findings: the statistical properties of some diatomic molecules like H_2 , HCl, CO, and LiH can be solved using Euler-Maclaurin summation. The characteristic values of electronic constants used in this calculation are given in Table 1: From the table, we have the reduced mass m , the dissociation parameter η , the range parameter, and the breath of the potential well a . In order to deduce the statistical properties of the given molecules (diatomic), the maximum quantum number n_{max} was obtained for the diatomic potential in equation (10), (q -deformed hyperbolic Pöschl-Teller potential), which is depicted in Table 2. $1 \text{ amu} = 931.5 \times 10^6 \text{ eV}(\text{\AA})$

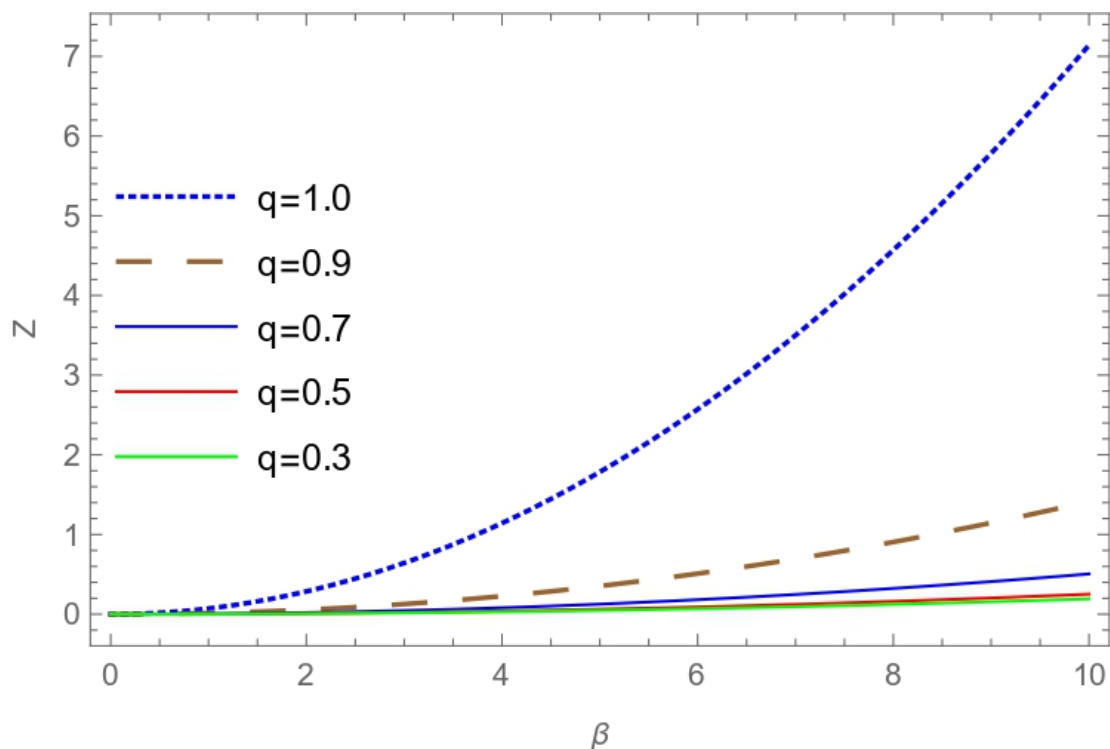


Figure 2. Disparity of q-deformed hyperbolic modified Pöschl-Teller partition function for distinct values of q (0<q<1).

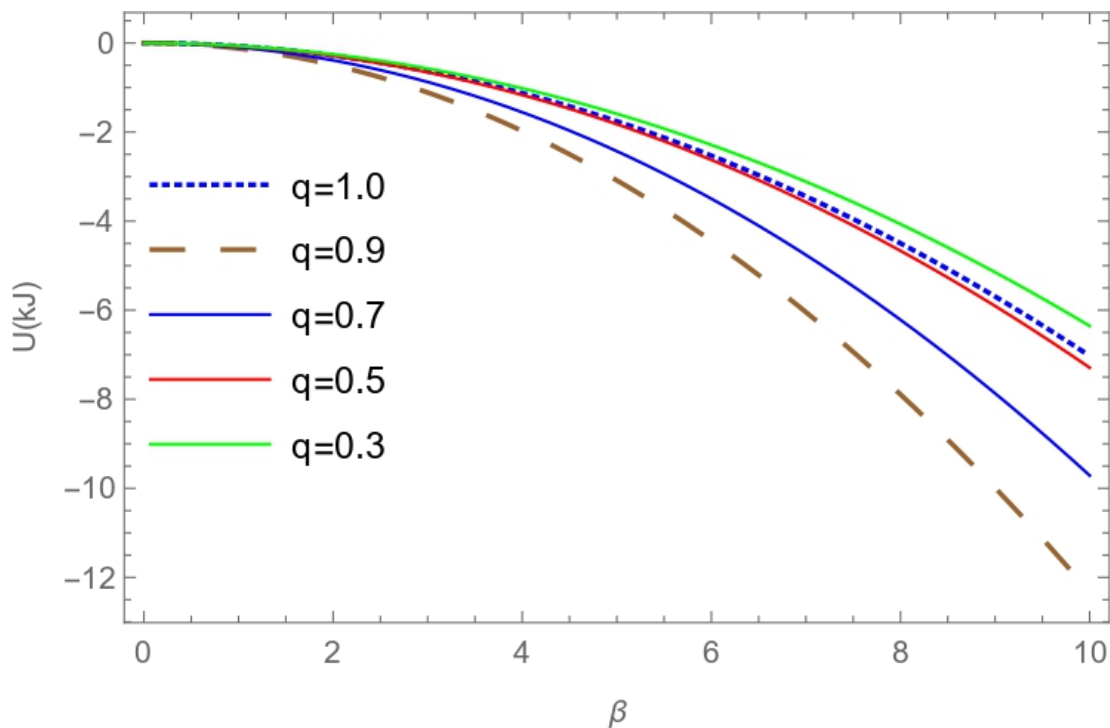


Figure 3. Disparity of q-deformed hyperbolic modified Pöschl-Teller vibrational internal energy for distinct values of q (0<q<1).

and $\hbar c = 1973.269 \text{ eV}(\text{\AA}^{-1})$ are used in obtaining the thermodynamic properties of the potential.

Figure 1 shows the variation of the potential for the distinct values of q with $0 < q < 1$ for the range value of r, from -5

to 20. It reveals that the deformation parameter q has a noticeable consequence on the depth of the potential. Figure 2 depicts the partition function (Z) of the potential for different values of Boltzmann factor (β) from 0 to 5. It reveals that vibrational par-

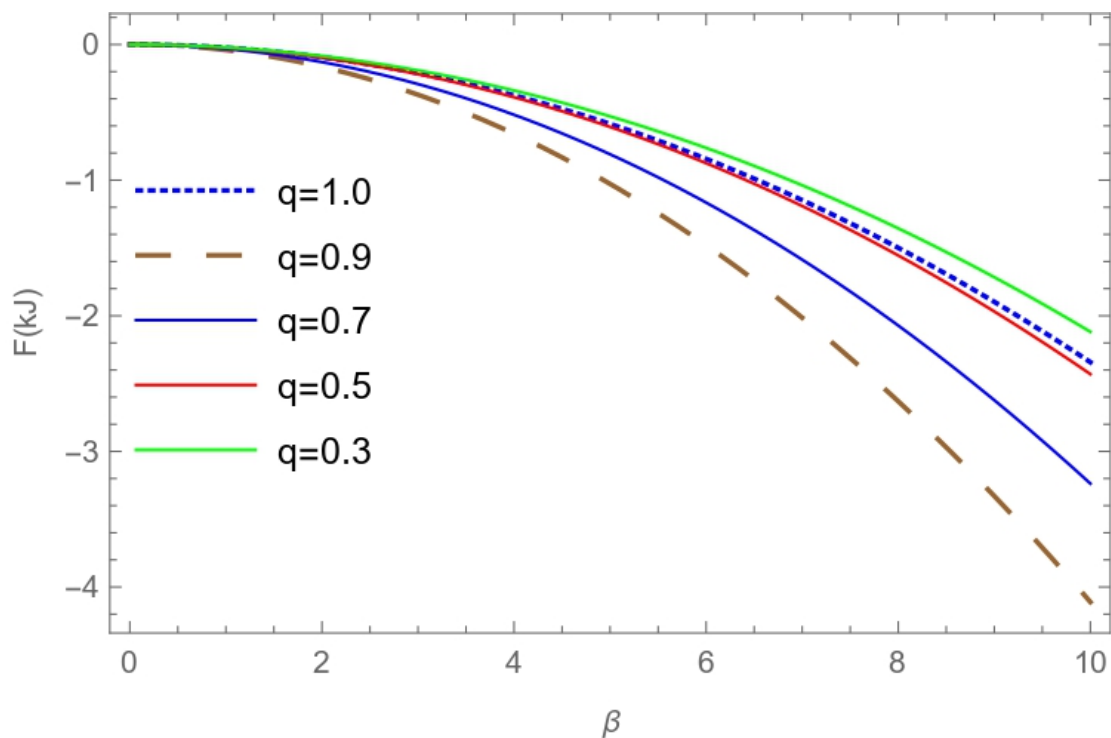


Figure 4. Disparity of q -deformed hyperbolic modified Pöschl-Teller vibrational free energy for distinct values of q ($0 < q < 1$).

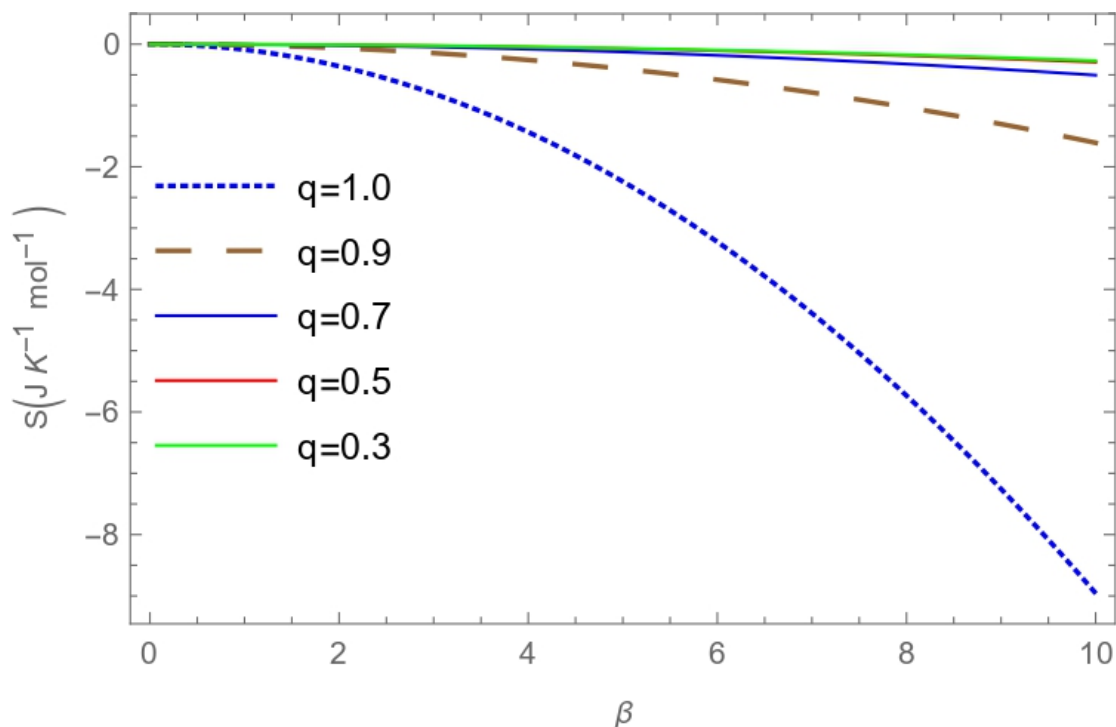


Figure 5. Disparity of q -deformed hyperbolic modified Pöschl-Teller vibrational entropy for distinct values of q ($0 < q < 1$).

tition function increases as Boltzmann factor (β) increases, and the greater the deformation parameter q , the greater the vibrational partition function. Figure 3 shows the q -deformed hyperbolic modified Pöschl-Teller molecular vibrational internal energy against different values of Boltzmann factor (β) from 0 to

5. It reveals that internal energy (U) increases as the Boltzmann factor (β), increases. The deformation parameter q has a significant effect on the vibrational internal energy of the system; the rise in deformation parameter q , the higher the instability of the diatomic molecules. Figure 4 shows the graph of vibrational

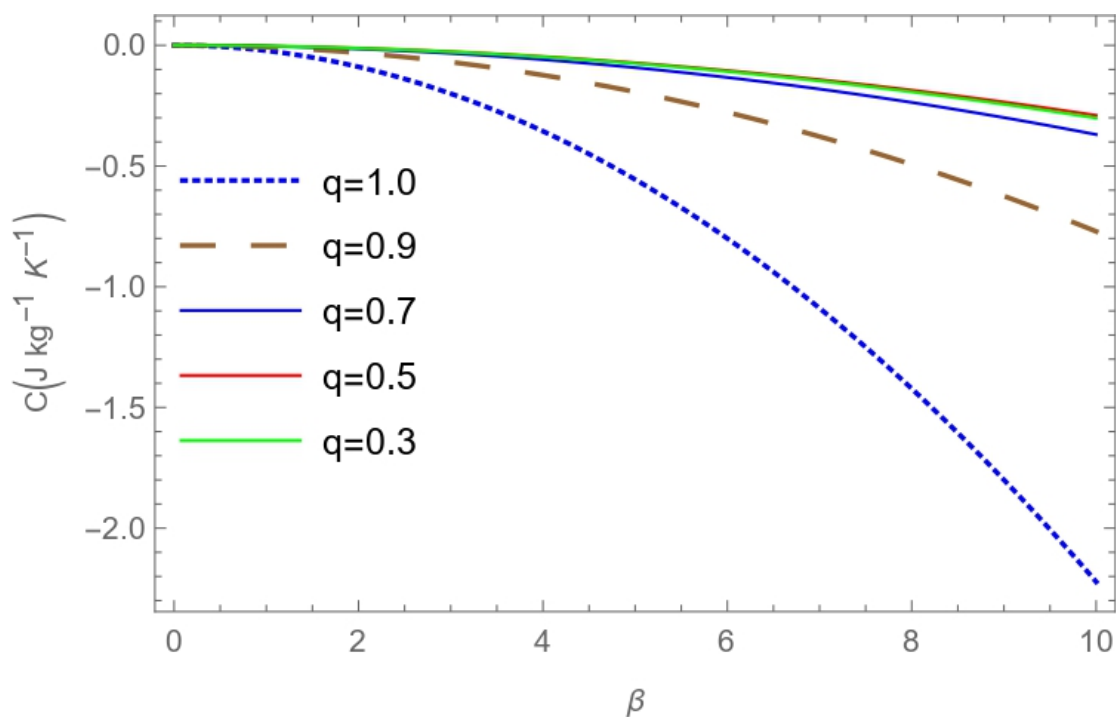


Figure 6. Disparity of q -deformed hyperbolic modified Pöschl-Teller vibrational specific heat capacity for distinct values of q ($0 < q < 1$).

Table 1. Disparity of q -deformed hyperbolic modified Pöschl-Teller vibrational specific heat capacity for distinct values of q ($0 < q < 1$).

Molecule	m (amu)	η (eV)	α (Å) ⁻¹	$a = \frac{1}{\alpha}$ (Å)
HCl	0.980104500	2.206600000	2.380570000	0.420067463
H ₂	0.503910000	2.234860000	1.440558000	0.694175451
CO	6.860671900	3.387570000	2.594410000	0.385444089
LiH	0.880122100	1.662920000	1.799836800	0.555605930

Table 2. The number of n_{max} used.

q	H ₂	HCl	LiH	CO
1	1.092580	0.532021	0.513148	0.884832
0.9	1.170440	0.575003	0.554866	0.950195
0.7	1.375150	0.689278	0.665865	1.122500
0.5	1.696050	0.871181	0.842735	1.393550
0.3	2.305550	1.222470	1.184700	1.910230

free energy (F) against different values of Boltzmann factor (β) from 0 to 5. It reveals that an increase in vibrational free energy (F) causes an increase in Boltzmann factor (β). The higher the deformational parameter q , the higher the free movement of the particle in the molecules. Figure 5 shows the variation in q -deformed hyperbolic modified Pöschl-Teller molecular entropy against Boltzmann factor (β) from 0 to 5. It reveals that an increase in entropy causes an increase in Boltzmann factor (β). The higher the deformation parameter q , the higher the level of

disorderliness of a system.

Figure 6 shows the heat capacity of the q -deformed modified Pöschl-Teller potential against change in different values of Boltzmann factor (β). It reveals that as the Boltzmann factor increases, the specific heat capacity of diatomic particles decreases. Furthermore, it is well observed that the specific heat capacity is highly sensitive to n_{max} than the partition function. The second derivative of the partition function gives the specific heat capacity, and the amplitude of the specific heat capacity as

a function of q is evident in Figure 6 for diatomic molecule. This enlargement can be explained by a monotonical decrease in n_{max} when q increases. It is due to state formation of the algebraic model, which simply means for a system of diatomic molecules of energy spectrum whose potential is q -deformed hyperbolic modified Pöschl-Teller potential, at a critical temperature the system becomes saturated in which all its excited states have been completely filled up. Figure 6 shows the behaviour of the specific heat capacity for HCl molecules with varying values of q . It is clearly shown that the specific heat capacity is almost the same in all cases of q . That is, the deformation parameter q does not have much significant effect on the transition phase and its nature on diatomic molecules.

4. Conclusion

The solution of the potential for the Schrödinger equation has been obtained analytically. We also compared the eigenvalues obtained from the Schrödinger equation at $l = 0$ and the result obtained with the literature for the case $l = 0$, for the s -wave state of the potential in the non-relativistic reference frame. The results are in excellent agreement. We have also achieved, from the vibrational partition function, various thermodynamic properties, that is, vibrational free energy, vibrational internal energy, vibrational entropy and vibrational specific capacity for the potential model. From the graphs of the thermodynamic properties with β , We noticed that vibrational internal energy, vibrational free energy, and vibrational entropy grow tediously with rise in β while the specific heat capacity falls with rise in β . Finally, We have analyzed the behaviour of the specific heat: this analysis shows the existence of a critical temperature, T_C , in the curves of the specific heat: this temperature decreases when increases, and we also discovered that T_C depends on the molecular weight, band length, and the vibrational frequency.

Data availability

We do not have any research data outside the submitted manuscript file.

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